

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 24 25 26
27

ring bonds :

1-2 1-6 2-3 2-19 3-4 3-22 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12
12-13 12-15 13-14 13-18 15-16 16-17 17-18 17-27 18-26 19-20 19-25 20-21 20-24
21-22

exact/norm bonds :

2-19 3-22 5-7 6-10 7-8 9-10 12-15 13-18 15-16 16-17 17-18 17-27 18-26 19-20
19-25 20-21 20-24 21-22

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-11 9-14 11-12 12-13 13-14

G1:C,N

G2:C,O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 24:Atom 25:Atom 26:Atom 27:Atom

=> d his

(FILE 'HOME' ENTERED AT 14:18:15 ON 03 FEB 2003)

FILE 'REGISTRY' ENTERED AT 14:18:23 ON 03 FEB 2003

L1 STRUCTURE UPLOADED

L2 1 S L1

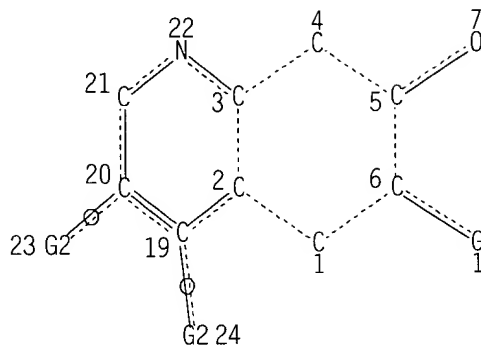
L3 40 S L1 FULL

=> d que 13 stat

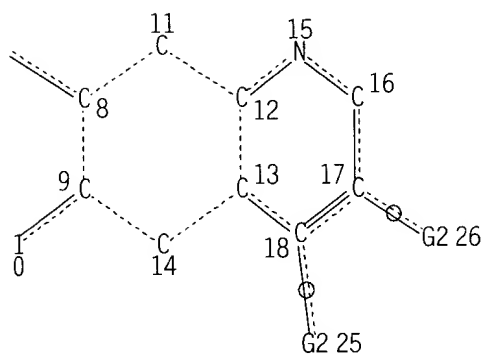
L1 STR

C 29 O 30 S 31 N 32

C 27 N 28



Page 1-A



Page 1-B

VAR G1=27/28

VAR G2=29/30/31/32

NODE ATTRIBUTES:

NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7

NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10
NSPEC IS R AT 11
NSPEC IS R AT 12
NSPEC IS R AT 13
NSPEC IS R AT 14
NSPEC IS R AT 15
NSPEC IS R AT 16
NSPEC IS R AT 17
NSPEC IS R AT 18
NSPEC IS R AT 19
NSPEC IS R AT 20
NSPEC IS R AT 21
NSPEC IS R AT 22
NSPEC IS R AT 23
NSPEC IS R AT 24
NSPEC IS R AT 25
NSPEC IS R AT 26

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

L3 40 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 8075 ITERATIONS

40 ANSWERS

SEARCH TIME: 00.00.01

=> fil capl

FILE 'CAPLUS' ENTERED AT 14:19:31 ON 03 FEB 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 3 Feb 2003 VOL 138 ISS 6

FILE LAST UPDATED: 2 Feb 2003 (20030202/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'FIONA' IS DEFAULT FORMAT FOR 'CAPLUS' FILE

=> s 13

L4 2 L3

=> d 1-2 ibib iabs hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:122962 CAPLUS

DOCUMENT NUMBER: 136:163717

TITLE: Novel hydroxyquinoline derivative fluorescent dyes and their biological applications

INVENTOR(S): Diwu, Zhenjun; Liu, Jiaying; Haugland, Richard P.; Gee, Kyle R.

PATENT ASSIGNEE(S): Molecular Probes, Inc., USA

SOURCE: PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2002012195	A1	20020214	WO 2001-US24479	20010804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001079185	A5	20020218	AU 2001-79185	20010804
US 2002059684	A1	20020523	US 2001-922333	20010804
PRIORITY APPLN. INFO.:			US 2000-223086P	P 20000804
			WO 2001-US24479	W 20010804

OTHER SOURCE(S): MARPAT 136:163717

ABSTRACT:

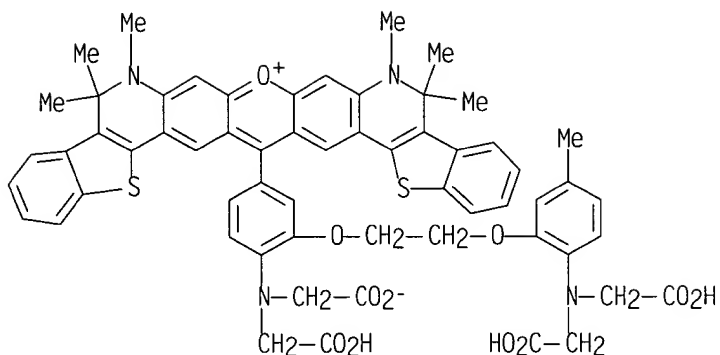
The present invention describes novel dyes, including coumarins, rhodamines, and rhodols that incorporate addnl. fused arom. rings. The dyes of the invention absorb at a longer wavelength than structurally similar dyes that do not possess the fused arom. rings. Many of the dyes of the invention are useful fluorescent dyes. The invention includes chem. reactive dyes, dye-conjugates, and the use of such dyes in staining samples and detecting ligands or other analytes.

IT 397883-14-6P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(novel hydroxyquinoline deriv. fluorescent dyes and biol. applications)

RN 397883-14-6 CAPLUS

CN Bis[1]benzothieno[3,2-c:3'.2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium, 18-[4-[bis(carboxymethyl)amino]-3-[2-[2-[bis(carboxymethyl)amino]-5-methylphenoxy]ethoxy]phenyl]-5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-, inner salt (9CI) (CA INDEX NAME)

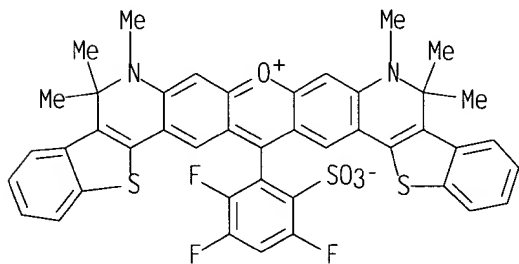


IT 397882-80-3P 397882-81-4P 397882-82-5P
 397882-83-6P 397882-85-8P 397882-87-0P
 397882-88-1P 397882-89-2P 397882-90-5P
 397882-91-6P 397882-92-7P 397882-99-4P
 397883-00-0P 397883-02-2P 397883-03-3P
 397883-05-5P 397883-06-6P 397883-07-7P
 397883-12-4P 397883-15-7P 397883-19-1P
 397883-20-4P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (novel hydroxyquinoline deriv. fluorescent dyes and biol. applications)

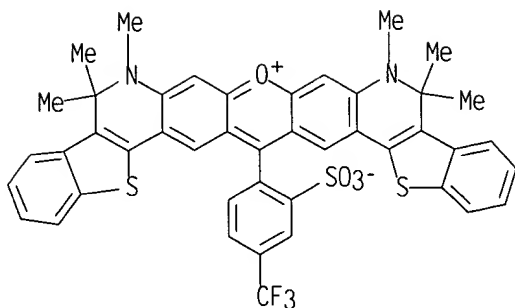
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CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinoln-8-ium,
 5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-18-(2,3,5-trifluoro-6-
 sulfo-phenyl)-, inner salt (9CI) (CA INDEX NAME)



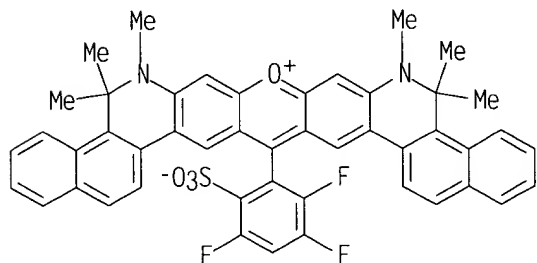
RN 397882-81-4 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinoln-8-ium,
 5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-18-[2-sulfo-4-
 (trifluoromethyl)phenyl]-, inner salt (9CI) (CA INDEX NAME)



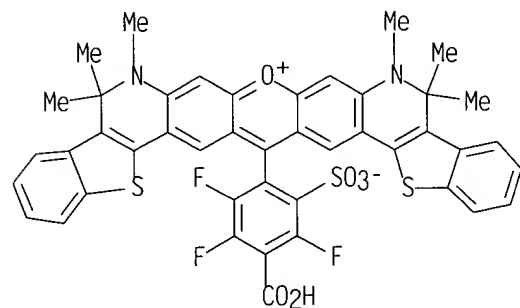
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5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-19-(2,3,5-trifluoro-6-
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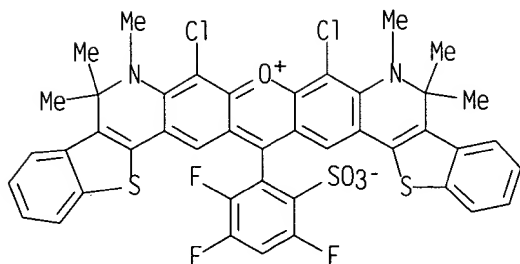
RN 397882-83-6 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
18-(4-carboxy-2,3,5-trifluoro-6-sulfohenyl)-5,6,10,11-tetrahydro-
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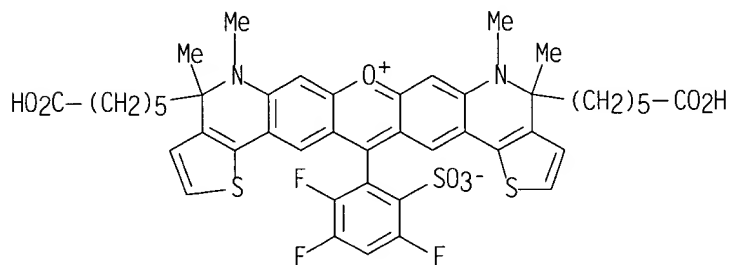
RN 397882-85-8 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
7,9-dichloro-5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-18-(2,3,5-
trifluoro-6-sulfohenyl)-, inner salt (9CI) (CA INDEX NAME)



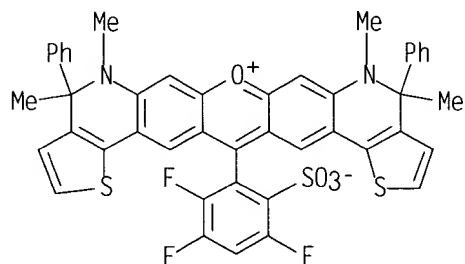
RN 397882-87-0 CAPLUS

CN Dithieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
4,10-bis(5-carboxypentyl)-4,5,9,10-tetrahydro-4,5,9,10-tetramethyl-15-
(2,3,5-trifluoro-6-sulphophenyl)-, inner salt (9CI) (CA INDEX NAME)



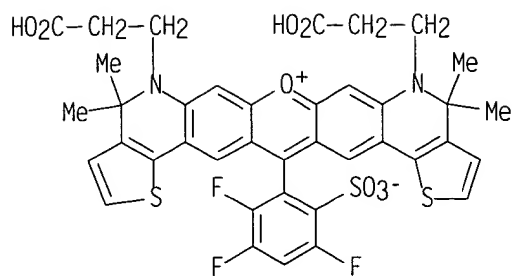
RN 397882-88-1 CAPLUS

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4,5,9,10-tetrahydro-4,5,9,10-tetramethyl-4,10-diphenyl-15-(2,3,5-trifluoro-
6-sulphophenyl)-, inner salt (9CI) (CA INDEX NAME)



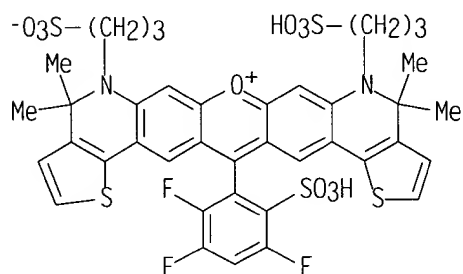
RN 397882-89-2 CAPLUS

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5,9-bis(2-carboxyethyl)-4,5,9,10-tetrahydro-4,4,10,10-tetramethyl-15-
(2,3,5-trifluoro-6-sulphophenyl)-, inner salt (9CI) (CA INDEX NAME)



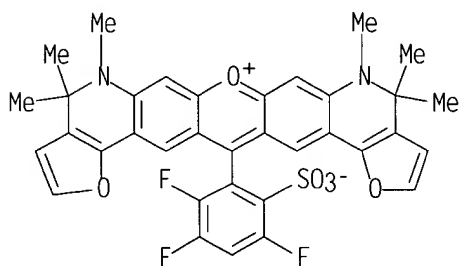
RN 397882-90-5 CAPLUS

CN Dithieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
4,5,9,10-tetrahydro-4,4,10,10-tetramethyl-5,9-bis(3-sulfopropyl)-15-(2,3,5-trifluoro-6-sulfophenyl)-, inner salt (9CI) (CA INDEX NAME)



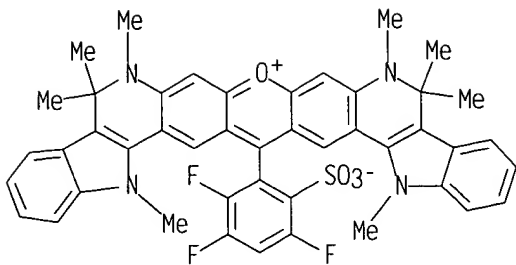
RN 397882-91-6 CAPLUS

CN Difuro[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-15-(2,3,5-trifluoro-6-sulfophenyl)-, inner salt (9CI) (CA INDEX NAME)



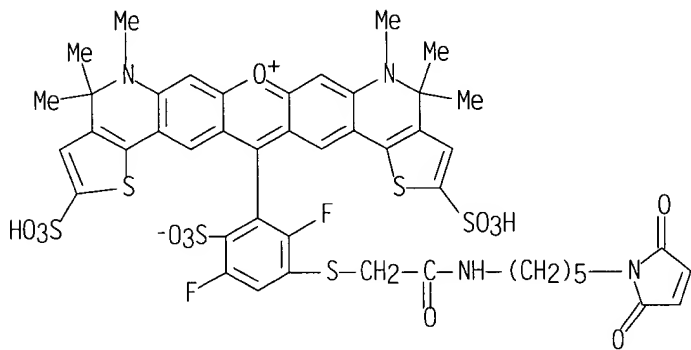
RN 397882-92-7 CAPLUS

CN Diindolo[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
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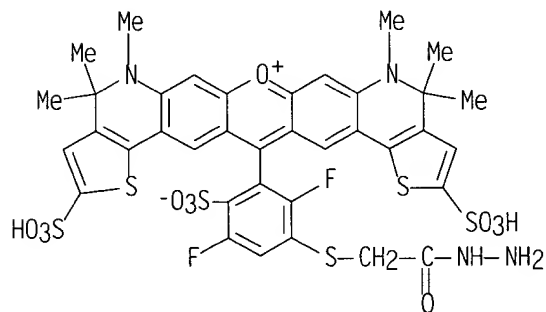
RN 397882-99-4 CAPLUS

CN Dithieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
15-[3-[[2-[[5-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)pentyl]amino]-2-oxoethyl]thio]-2,5-difluoro-6-sulphophenyl]-4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-2,12-disulfo-, inner salt (9CI) (CA INDEX NAME)



RN 397883-00-0 CAPLUS

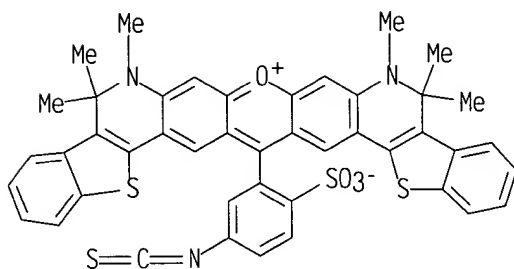
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15-[2,5-difluoro-3-[(2-hydrazino-2-oxoethyl)thio]-6-sulphophenyl]-4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-2,12-disulfo-, inner salt (9CI) (CA INDEX NAME)



RN 397883-02-2 CAPLUS

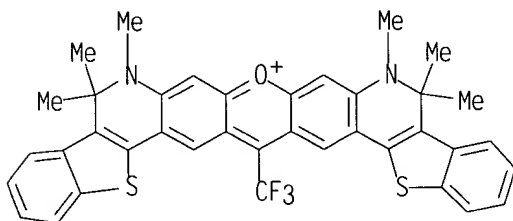
CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
5,5,6,10,11-tetrahydro-18-(5-isothiocyanato-2-sulphophenyl)-5,5,6,10,11,11-

hexamethyl-, inner salt (9CI) (CA INDEX NAME)



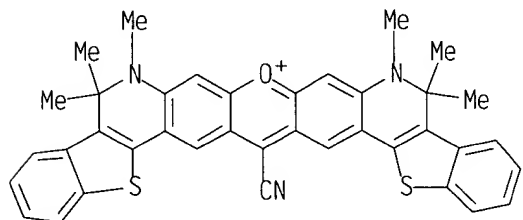
RN 397883-03-3 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-18-(trifluoromethyl)-,
inner salt (9CI) (CA INDEX NAME)



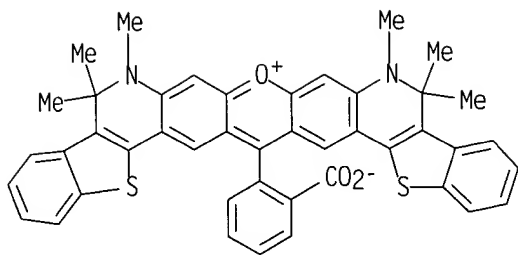
RN 397883-05-5 CAPLUS

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NAME)



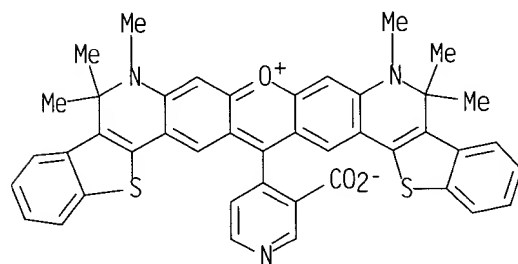
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CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
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inner salt (9CI) (CA INDEX NAME)



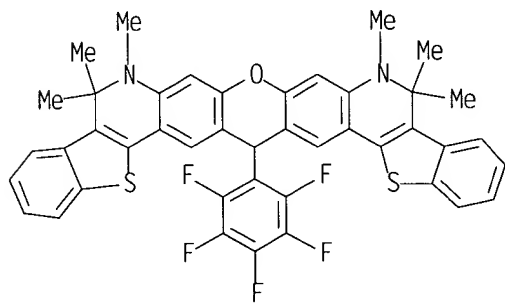
RN 397883-07-7 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
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, inner salt (9CI) (CA INDEX NAME)



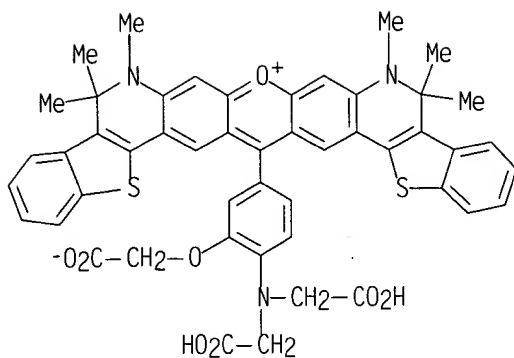
RN 397883-12-4 CAPLUS

CN 5H-Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinoline,
6,10,11,18-tetrahydro-5,5,6,10,11,11-hexamethyl-18-(pentafluorophenyl)-
(9CI) (CA INDEX NAME)



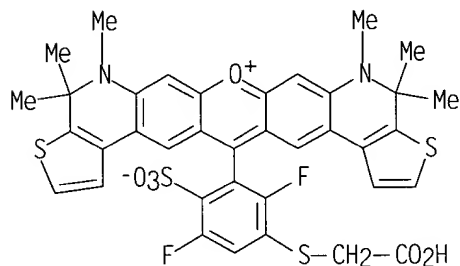
RN 397883-15-7 CAPLUS

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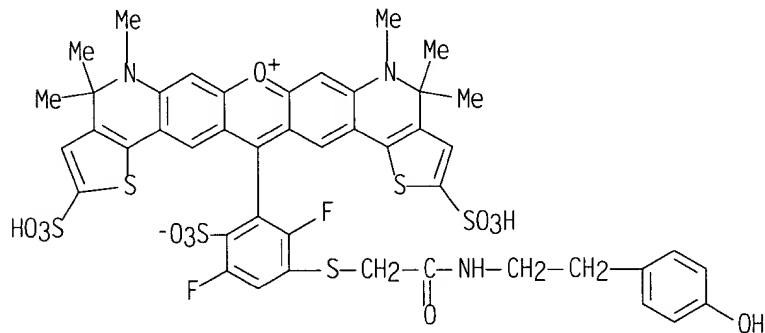
RN 397883-19-1 CAPLUS

CN Dithieno[2,3-c:2',3'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
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tetrahydro-4,4,5,9,10,10-hexamethyl-, inner salt (9CI) (CA INDEX NAME)



RN 397883-20-4 CAPLUS

CN Dithieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
15-[2,5-difluoro-3-[[2-[[2-(4-hydroxyphenyl)ethyl]amino]-2-oxoethyl]thio]-
6-sulfo-phenyl]-4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-2,12-disulfo-,
inner salt (9CI) (CA INDEX NAME)



IT 397882-79-0P 397882-84-7P 397882-96-1P
397882-97-2P 397882-98-3P 397883-01-1P
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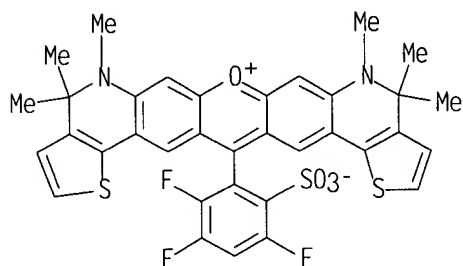
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(novel hydroxyquinoline deriv. fluorescent dyes and biol. applications)

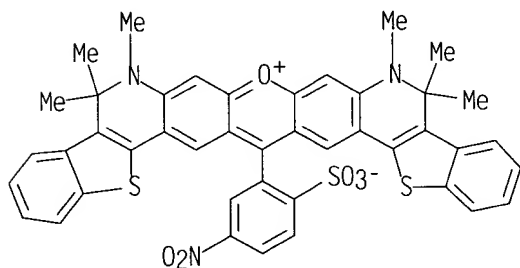
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CN Dithieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinol-7-ium,
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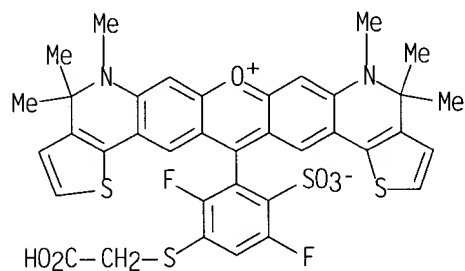
RN 397882-84-7 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinol-8-ium,
5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-18-(5-nitro-2-sulfo-phenyl)-, inner salt (9CI) (CA INDEX NAME)



RN 397882-96-1 CAPLUS

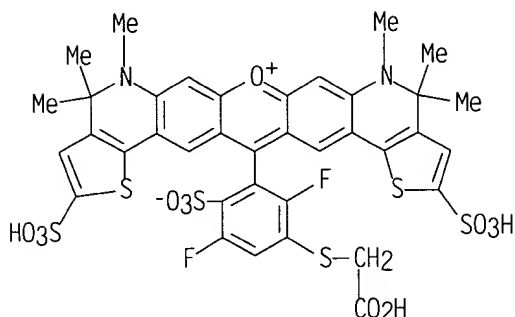
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15-[3-[(carboxymethyl)thio]-2,5-difluoro-6-sulfo-phenyl]-4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-, inner salt (9CI) (CA INDEX NAME)



RN 397882-97-2 CAPLUS

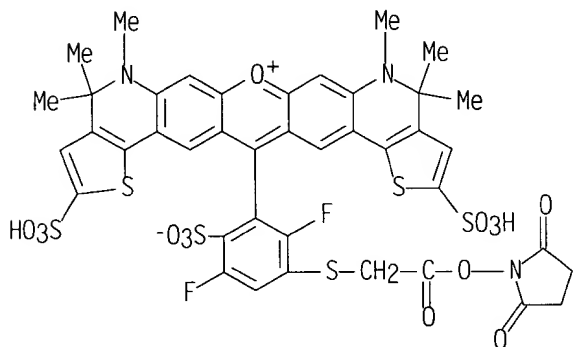
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15-[3-[(carboxymethyl)thio]-2,5-difluoro-6-sulfo-phenyl]-4,5,9,10-

tetrahydro-4,4,5,9,10,10-hexamethyl-2,12-disulfo-, inner salt (9CI) (CA INDEX NAME)



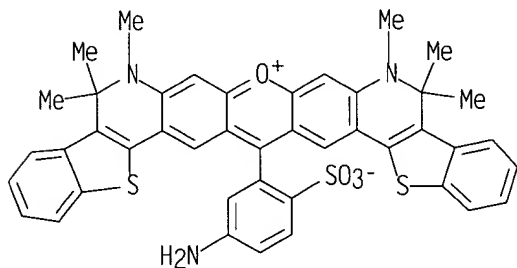
RN 397882-98-3 CAPLUS

CN Dithieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-7-ium,
15-[3-[[2-[(2,5-dioxo-1-pyrrolidinyloxy)-2-oxoethyl]thio]-2,5-difluoro-6-
sulphophenyl]-4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-2,12-disulfo-,
inner salt (9CI) (CA INDEX NAME)



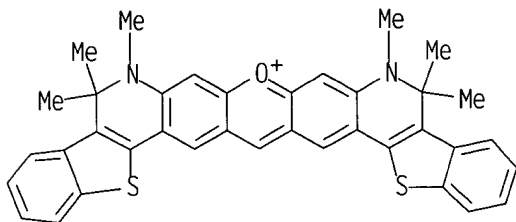
RN 397883-01-1 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolin-8-ium,
18-(5-amino-2-sulphophenyl)-5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-
, inner salt (9CI) (CA INDEX NAME)



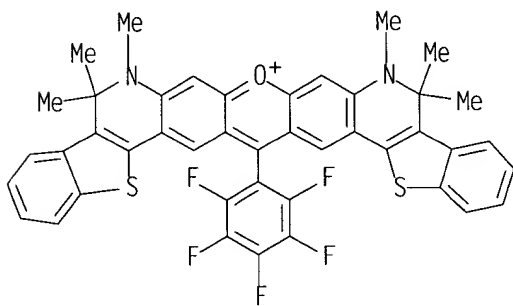
RN 397883-04-4 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolín-8-ium.
5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl- (9CI) (CA INDEX NAME)



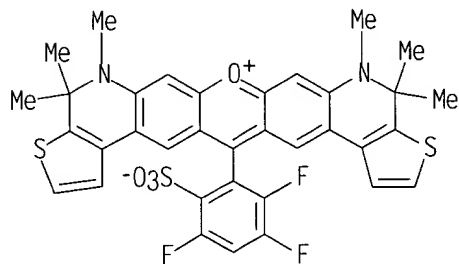
RN 397883-11-3 CAPLUS

CN Bis[1]benzothieno[3,2-c:3',2'-c']pyrano[3,2-g:5,6-g']diquinolín-8-ium.
5,6,10,11-tetrahydro-5,5,6,10,11,11-hexamethyl-18-(pentafluorophenyl)-
(9CI) (CA INDEX NAME)



RN 397883-18-0 CAPLUS

CN Dithieno[2,3-c:2',3'-c']pyrano[3,2-g:5,6-g']diquinolín-7-ium,
4,5,9,10-tetrahydro-4,4,5,9,10,10-hexamethyl-15-(2,3,5-trifluoro-6-
sulfophenyl)-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:434239 CAPLUS
DOCUMENT NUMBER: 133:71117
TITLE: The synthesis of 4,7-Dichlororhodamine dyes and their
use in polynucleotide sequencing and fragment analysis
INVENTOR(S): Lee, Linda; Benson, Scott C.; Rosenblum, Barnett B.;
Spurgeon, Sandra L.
PATENT ASSIGNEE(S): The Perkin-Elmer Corporation, USA
SOURCE: U.S., 16 pp., Cont.-in-part of U.S. Ser. No. 38,191.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6080852	A	20000627	US 1999-277793	19990327
US 5847162	A	19981208	US 1996-672196	19960627
US 6025505	A	20000215	US 1998-38191	19980310
WO 2000058406	A1	20001005	WO 2000-US8003	20000324
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1165694 A1 20020102 EP 2000-916662 20000324 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO JP 2002540280 T2 20021126 JP 2000-608692 20000324 PRIORITY APPLN. INFO.: US 1996-672196 A2 19960627 US 1998-38191 A2 19980310 US 1999-277793 A 19990327 WO 2000-US8003 W 20000324 OTHER SOURCE(S): MARPAT 133:71117 GRAPHIC IMAGE:				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

ABSTRACT:

A set of 4,7-dichlororhodamine compds. useful as fluorescent dyes are disclosed having the structures (I) and (II); wherein R1 -R6 are hydrogen, fluorine, chlorine, lower alkyl, lower alkene, lower alkyne, sulfonate, sulfone, amino, amido, nitrite, lower alkoxy, linking group, or, when taken together, R1 and R6 is benzo, or, when taken together, R4 and R5 is benzo; R7 -R10, R12 -R16 and R18 may be hydrogen, fluorine, chlorine, lower alkyl, lower alkene, lower

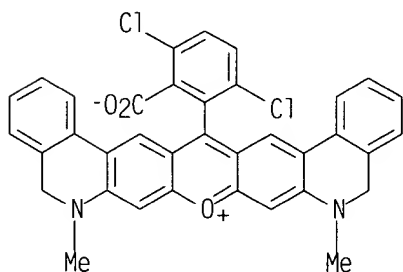
alkyne, sulfonate, sulfone, amino, amido, nitrite, lower alkoxy, linking group; R11 and R17 may be hydrogen, lower alkyl, lower alkene, lower alkyne, Ph, aryl, linking group; Y1 -Y4 are hydrogen, lower alkyl, or cycloalkyl, or, when taken together, Y1 and R2, Y2 and R1 Y3 and R3, and/or Y4 and R4 is propano, ethano, or substituted forms thereof, and X1 -X3 taken sep. are hydrogen, chlorine, fluorine, lower alkyl, carboxylate, sulfonate, hydroxymethyl, and linking group, or any combinations thereof. In another aspect, the invention includes reagents labeled with the 4,7-dichlororhodamine dye compds., including deoxynucleotides, dideoxynucleotides, and polynucleotides. In an addnl. aspect, the invention includes methods utilizing such dye compds. and reagents including dideoxy polynucleotide sequencing and fragment anal. methods.

IT **278180-72-6P**

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(the synthesis of 4,7-Dichlororhodamine dyes and their use in polynucleotide sequencing and fragment anal.)

RN 278180-72-6 CAPLUS

CN Pyrano[3,2-b:5,6-b']diphenanthridin-8-ium, 17-[2,4(or 2.5)-dicarboxy-3,6-dichlorophenyl]-5,6,10,11-tetrahydro-6,10-dimethyl-, inner salt (9CI) (CA INDEX NAME)



D1-CO₂H

REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT